

Degradation of dental resin through water diffusion

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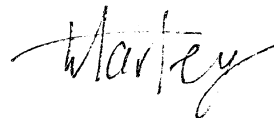
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Introduction

Dental resin is used in the dentistry field as restorative material that fills out cavity of teeth. It is insoluble, aesthetic, unreactive in dehydration, and inexpensive which makes it a very reasonable option for patients who want their cavity to be cured in a more aesthetic way. Dental resin is mainly composed of two polymers called Bis-GMA and TEGMA. However, with time, these resins do not last due to environmental issues. Most of the water molecules that penetrate inside the resin is saliva. These molecules go through all the way down into the gap between the dentin and resin. As water molecules accumulate between these gaps, resins start to fall apart slowly and eventually separates completely from the dentin.

Literature Review

Water diffusion into dental resin accelerates the rate of degradation. Epoxy polymer prevents corrosion when it interacts with water molecules, but it falls apart due to moisture adsorbed by the resin (Pandiyan). As the higher the amount of water, the higher the plasticity of the epoxy polymer (Pandiyan). The paper used computational software which is GROMACS to set up the simulation. We are also using GROMACS for research on water diffusion. EPON-828 and DETA (Diethylenetriamine) molecules were used and OPLS-AA force field parameters used (Pandiyan). 215 EPON-828 and 86 DETA looked for closest neighbors and formed limited number of cross-linked bonds. Energy minimization was performed to have equilibrium in the mixture. At the final conversion, about 99% of the chains (213 epoxy chains and 86 DETA molecules) in the simulation box were involved in a single network structure (Pandiyan).

According to **Figure 1**, as the conversion increases, the size of the epoxy clusters becomes bigger and there is a sharp change of the size of epoxy cluster between the conversion = 0.4 and 0.5. For the valid epoxy network model, the cross link conversion between epoxy molecules is limited to 0.4.

Method

Computational simulation uses a software program to model molecules that will be used for simulation. To experiment with water diffusion into dental resin, polymers of Bisphenol-A glyceril methacrylate (Bis-GMA) and Triethylene glycol dimethacrylate (TEGDMA) were created through CERIU2. These two polymers run energy minimization using a Dreiding force field in order to offer a stable environment for water molecules to diffuse. The ratio of Bis-GMA and TEGDMA was 50:50. Time for energy minimization was 500ps, temperature was 310K, pressure was 1 atm and density was 0.99g/cm³. Molecular Dynamic (MD) simulation is the method used to calculate the motion of the molecules in a molecular assembly by using Newtonian dynamics to determine the net force and acceleration that is experienced by each atom. Monomer Complex in equilibrium of two polymers will be achieved. As shown in **Figure 2**, red indicates TEGDMA, blue indicates Bis-GMA and Green indicates Photo-initiator which is also known as DMAEMA. Water molecules were created also using Cerius2.

Result

Complex monomers of Bis-GMA, TEGDMA, DMAEMA and water molecules cross linked.

Figure 4 shows how each monomer cross linked and formed one core structure of dental resin.

After putting water molecules inside the complex monomer structure of dental resin, it undergo

equilibrium to have the most stable condition so that water molecules attach to resin polymer. As shown in **Figure 2**, the initial dimension of the resin structure was $45 \times 45 \times 45 \text{ \AA}^3$. However, as shown in **Figure 3**, it changed to $46.3 \times 46.3 \times 46.3 \text{ \AA}^3$ after equilibrium. As the dimensions changed, energy and volume were affected. **Figure 5** shows that total energy was stabilized as time passed. The red line in **Figure 6** represents the initial volume before equilibrium. As shown in **Figure 6**, the volume increased up to 108000 \AA^3 and stabilized around 100000 \AA^3 after equilibrium. Radial distribution function was performed to determine the probability of finding a particle at a distance of r away from a chosen reference point or particle. As shown in **Figure 7**, three atoms were selected in BisGMA, and RDF was performed to investigate the distribution of water molecules around BisGMA. In **Figure 8**, the distance which is shown as green between water molecules and oxygen 1 is the shortest which is approximately 3.5 \AA . Water molecules are staying the closest to oxygen 1 atom.

Discussion

The volume and energy were increased after equilibrium. Volume increased in order to have more empty spaces between monomers that allowed water molecules to get into those spaces. Also, energy was increased in order to make the resin structure as the most stable condition. After analyzing RDF distribution, Bis-GMA have water molecules at around 3.5 \AA . This implies that TEGDMA would have water molecules closer than 3.5 \AA since Bis-GMA is a hydrophobic monomer. This can be seen from **Figure 3** where most of water molecules are attached with red monomers which are TEGDMA.

Conclusions

Complex monomers of Bis-GMA, TEGDMA, DMAEMA and water molecules cross linked each other. They formed one core structure of dental resin with water molecules inside. They reached a state of equilibrium by increasing dimensions in length, height and width, volume and energy. Volume increased in order to allow more water molecules to reside in empty spaces between monomers. Additionally, energy increased in order to reach the stable condition. Since Bis-GMA is a hydrophobic monomer, it does not attract water molecules as TEGDMA which is hydrophilic monomer.

Future work

Same simulations that was held previously can be run again with various mass of water. In order to see the relationship between the mass percent of water and change of volume, the mass of water will be constantly increased in each experiment.

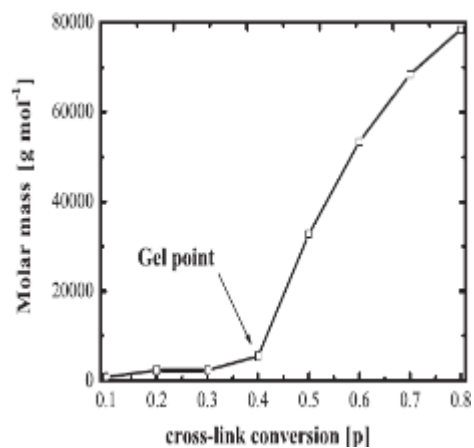


Figure 1. As the conversion increases, the size of the epoxy clusters becomes bigger.

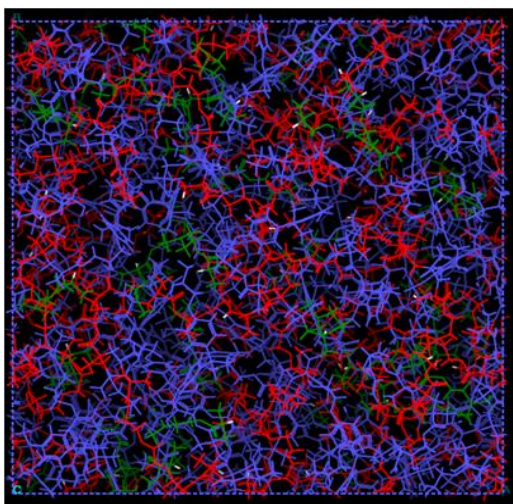


Figure 2. Red indicates TEGDMA, blue indicates Bis-GMA and Green indicates Photoinitiator which is also known as DMAEMA. Initial dimension 45 x 45 x 45 Å³.

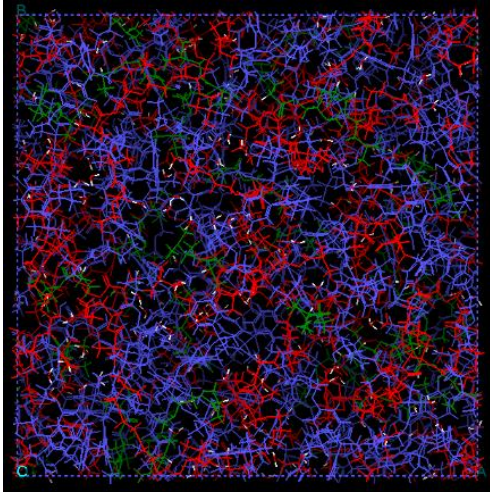


Figure 3. Dimension, $46.3 \times 46.3 \times 46.3 \text{ \AA}^3$, after equilibrium

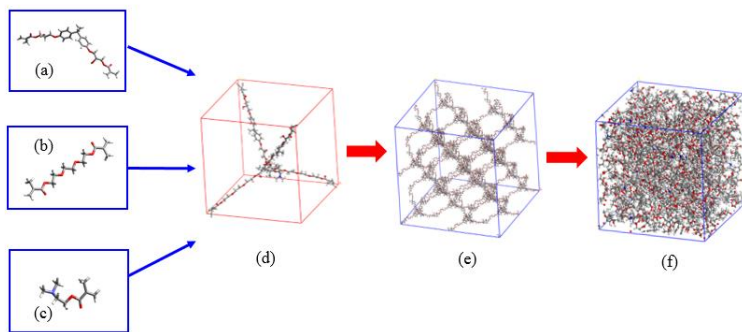


Figure 4. (a) indicates Bis-GMA, (b) indicates TEDGMA and (c) indicates DMAEMA.

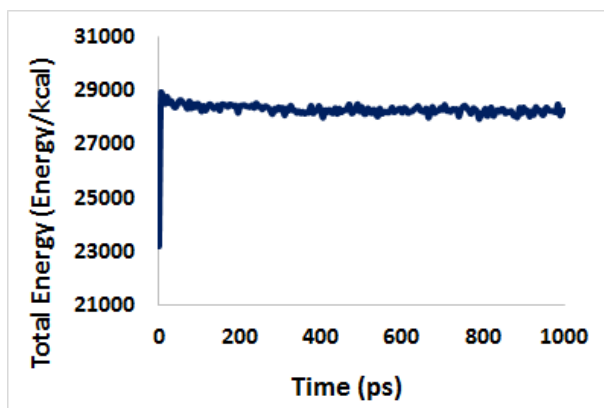


Figure 5. Time vs Total Energy graph after equilibrium

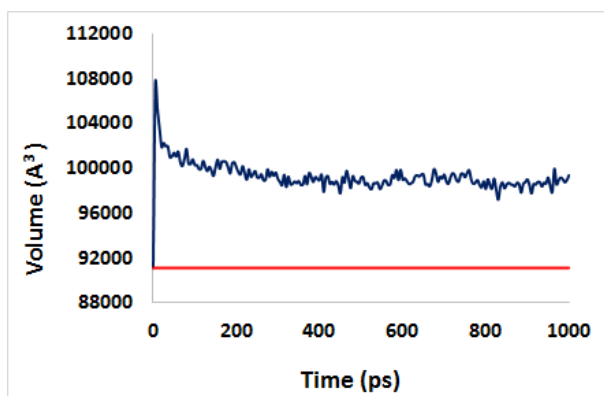


Figure 6. Time vs Volume graph after equilibrium

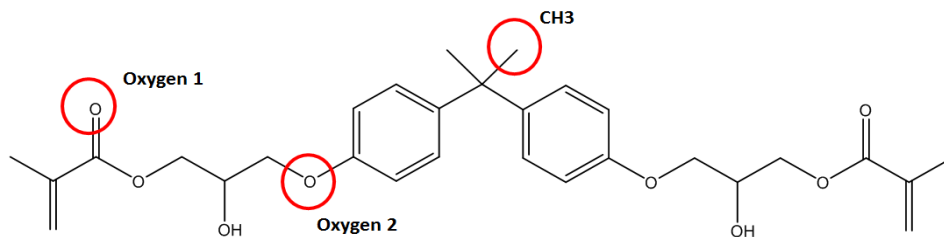


Figure 7. Water Distribution (5%) around BisGMA

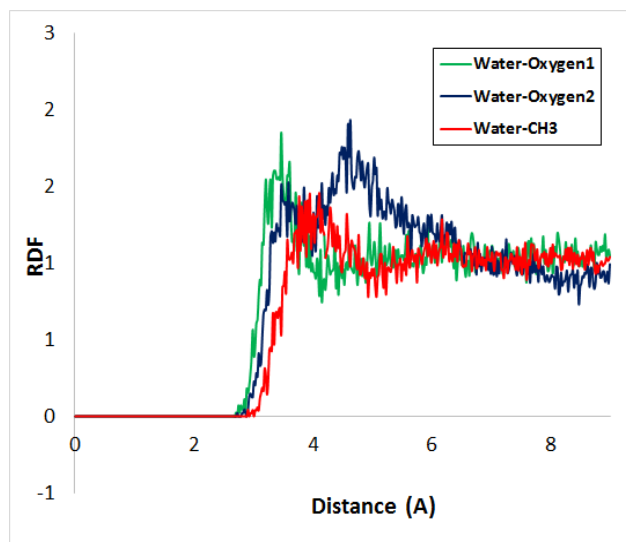


Figure 8. RDF vs Distance graph

Reference

Pandiyan, Sudharsan. *A Molecular Dynamics Study of Water Transport Inside an Epoxy Polymer Matrix*. Web. 26 Apr. 2016.